

# Non-fragile superconductivity with nodes in the superconducting topological insulator $\text{Cu}_x\text{Bi}_2\text{Se}_3$ : Zeeman orbital field and non-magnetic impurities

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We study the robustness against non-magnetic impurities in the topological superconductor with point nodes, focusing on an effective model of  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ . We find that the topological superconductivity with point-nodes is not fragile against non-magnetic impurities, although the superconductivity with nodes in past studies is usually fragile. Exchanging the role of spin with the one of orbital, and vice versa, we find that in the “dual” space the topological superconductor with point-nodes is regarded as the intra-orbital spin-singlet  $s$ -wave one. From the viewpoint of the dual space, we deduce that the point-node state is not fragile against non-magnetic impurity, when the orbital imbalance in the normal states is small. Since the spin imbalance is induced by the Zeeman magnetic field, we shall name this key quantity for the impurity effects Zeeman “orbital” field. The numerical calculations support that the deduction is correct. If the Zeeman orbital field is small, the topological superconductivity is not fragile in dirty materials, even with nodes. Thus, the topological superconductors can not be simply regarded as one of the *conventional* unconventional superconductors.

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The discovery of topological insulators [1–10] leads to a number of the studies about topological aspects in solid-state physics[11]. Topological superconductors[12] are of particular interest, since the emergence of the superconducting order is associated with the occurrence of a non-trivial topological invariant[3–5, 8]. In addition, they allow us to manipulate the Majorana fermion in materials and open an intriguing way of quantum engineering.

The quest for the bulk topological superconductors is an exciting issue in topological material science. The copper intercalated topological insulator  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  shows superconductivity at  $T_c \approx 3.8\text{K}$  and is a candidate for the bulk topological superconductors [12–15]. Identifying the gap-function type is now in great demand. The point-contact spectroscopy[16, 17] showed the zero-bias conductance peaks from the Majorana bound states at the surface edges. However, the scanning tunneling spectroscopy[18] indicated a fully-gapped feature in the density of states (DOS); there is no in-gap state, and therefore the superconducting state could be topologically trivial. In addition, the Knight-shift measurement[19] showed the presence of in-plane anisotropy. Hashimoto *et al.*[20] pointed out that the anisotropy is related to a character of a point-nodes gap function on  $a$ - $b$ -plane, since the electronic structure in the normal states is almost isotropic. The point-node gap function also induces the in-plane anisotropy of the thermal conductivity[21]. Fu [22] argued a different scenario for the in-plane anisotropy, using an odd-parity full gap state and the normal-state Hamiltonian with a hexagonal warping term of the spin-orbital coupling.

The possibility of the nodal gap function in  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  is very surprising and curious. Typically, this superconducting compound is considered to be dirty owing to the copper intercalated process. Indeed, the short mean-free path was reported experimentally[15]. A large number

of the studies about superconducting alloys[23–27] indicate that the superconductivity of an unconventional state (e.g.,  $d$ -wave and chiral  $p$ -wave) promptly diminishes via impurity scattering, different from the robustness of an  $s$ -wave state against non-magnetic impurities (Anderson’s theorem[23]). In particular, a nodal order is very fragile against non-magnetic impurities, since the low-energy excitations are produced around the nodes in the momentum space. Therefore, many questions arise: How does one understand the existence of a nodal superconducting state in the dirty materials? Is the topological superconductor with a point node really fragile against non-magnetic impurities?

In this paper, we study the robustness of a point-node gap function against non-magnetic impurities in an effective model for  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ . The model has the massive Dirac Hamiltonian in the normal part and the on-site pair potential in the superconducting part. We propose a simple and intuitive way of understanding the impurity effects of a point-node gap function. We focus on the spin and orbital degrees of freedom in the Bogoliubov-de Gennes (BdG) Hamiltonian. Exchanging the role of spin with the one of orbital, and vice versa, one can obtain a “dual” space with respect to the original space.

From the viewpoint of the dual space, we deduce that the point-node state is *not* fragile against non-magnetic impurity, when the orbital imbalance in the normal states is small. Since the spin imbalance is induced by the Zeeman magnetic field, we shall name this key quantity for the impurity effects Zeeman “orbital” field. We find that the Zeeman orbital field is connected with the mass of the Dirac Hamiltonian. Thus, the role of the Zeeman orbital field is qualitatively examined by measuring the amount of relativistic effects[28]. The numerical calculations of the DOS support that the deduction is correct. Using a self-consistent  $T$ -matrix approach for impurity scattering

with a unitary limit, we confirm that the in-gap states in the DOS are not induced, when the Zeeman orbital field is small (i.e., the normal-state stays at the relativistic regime). In addition, we show the importance of the Zeeman orbital field for the impurity effects of the point-node state in terms of the violation of Anderson's theorem, within the Born approximation. Thus, the topological superconductors can not be simply regarded as one of the *conventional* unconventional superconductors.

The mean-field Hamiltonian for  $\text{Cu}_x\text{Bi}_2\text{Se}_3$  is  $H = \int d^3\mathbf{k} \psi^\dagger(\mathbf{k}) \mathcal{H}(\mathbf{k}) \psi(\mathbf{k})$ . The 8-component column vector  $\psi(\mathbf{k})$  is composed of the electron annihilation ( $c_{\mathbf{k},\alpha}$ ) and creation operators ( $c_{\mathbf{k},\alpha}^\dagger$ ), where  $\alpha$  is a collective coordinate for orbital (1, 2) and spin ( $\uparrow, \downarrow$ );  $\psi(\mathbf{k}) = (c_{\mathbf{k},1,\uparrow}, c_{\mathbf{k},2,\uparrow}, c_{\mathbf{k},1,\downarrow}, c_{\mathbf{k},2,\downarrow}, c_{-\mathbf{k},1,\uparrow}^\dagger, c_{-\mathbf{k},2,\uparrow}^\dagger, c_{-\mathbf{k},1,\downarrow}^\dagger, c_{-\mathbf{k},2,\downarrow}^\dagger)^T$ . The  $8 \times 8$  matrix  $\mathcal{H}(\mathbf{k})$  is the BdG Hamiltonian matrix[21, 30–33],

$$\mathcal{H}(\mathbf{k}) = \begin{pmatrix} h_0(\mathbf{k}) & \Delta_{\text{pair}}(\mathbf{k}) \\ \Delta_{\text{pair}}^\dagger(\mathbf{k}) & -h_0^*(-\mathbf{k}) \end{pmatrix}. \quad (1)$$

The normal-part effective Hamiltonian  $h_0$  is described by the massive Dirac Hamiltonian with the strong spin-orbital coupling and the negative Wilson mass term[30],

$$h_0(\mathbf{k}) = \epsilon(\mathbf{k}) s^0 \otimes \sigma^0 + h_z(\mathbf{k}) + h_{so}(\mathbf{k}), \quad (2)$$

with  $h_z(\mathbf{k}) = M(\mathbf{k}) s^0 \otimes \sigma^3$  and  $h_{so}(\mathbf{k}) = \sum_{i=1}^3 P_i(\mathbf{k}) s^i \otimes \sigma^1$ , where  $\sigma^i$  ( $s^i$ ) are the  $2 \times 2$  Pauli matrices in the orbital (spin) space. The identity matrix in each space is labeled by the superscript 0 ( $\sigma^0$  and  $s^0$ ). Within on-site interaction, the pair potential  $\Delta_{\text{pair}}$  must fulfill the relation  $\Delta_{\text{pair}}^T = -\Delta_{\text{pair}}$  owing to the fermionic property. We have six possible gap functions classified by a Lorentz-transformation property[21]; they are classified into a pseudo-scalar, a scalar, and a polar vector (four-vector). In this paper, we focus on a polar vector parallel to  $y$ -axis (so-called  $\Delta_4$ [12]) given as

$$\Delta_4 = \Delta s^0 \otimes \sigma^2, \quad (3)$$

motivated by a scenario for explaining the in-plane anisotropy in the Knight-shift measurement[20]. The excitation spectrum of this gap function has a point node on  $k_y$ -axis in the momentum space[21, 34, 35].

Now, we propose an intuitive way of understanding the impurity effects of a point-node gap function. Let us exchange the role of spin with the one of orbital, and vice versa, in the BdG Hamiltonian ( $s^\mu \leftrightarrow \sigma^\mu$ , with  $\mu = 0, 1, 2, 3$ ). In the dual space, the “spin” Pauli (and identity) matrices are written by  $\tilde{s}^\mu$ , where  $\tilde{s}^\mu = \sigma^\mu$ . Similarly, the “orbital” matrices are denoted by  $\tilde{\sigma}^\mu$ . In the dual space, the topological superconductor with point-nodes,  $\Delta_4$  is regarded as the intra-orbital spin-singlet  $s$ -wave pairing,

$$\Delta_4^{\text{dual}} = -i\Delta \tilde{\sigma}^0 \otimes i\tilde{s}^2. \quad (4)$$

The mass term  $h_z(\mathbf{k})$  induces the orbital imbalance into the system in the original space. In the dual space, this

term is regarded as a contribution inducing the spin imbalance into the system,  $h_z^{\text{dual}} = M(\mathbf{k}) \tilde{\sigma}^0 \otimes \tilde{s}^3$ . Summarizing the above arguments, we find that in the dual space the system has a spin-singlet state under the Zeeman magnetic field. Under the Zeeman magnetic field, the  $s$ -wave superconductors become fragile against non-magnetic impurities, since the spin imbalance due to the Zeeman magnetic field assists impurities with breaking Cooper pairs. However, when the Zeeman magnetic field is small, the  $s$ -wave state is robust against non-magnetic impurities, owing to Anderson's theorem, since the non-magnetic impurity is non-magnetic in the dual space. Therefore, we claim that the point-node state is not fragile against non-magnetic impurities in the weak Zeeman orbital field.

Before checking our statement with a more concrete way, we quantify the strength of the Zeeman orbital field suitable for studying the role in the impurity effects. For this purpose, we use  $\beta$  defined by

$$\beta \equiv \frac{|\mathbf{P}(\mathbf{k}_F)|}{|M(\mathbf{k}_F)|}, \quad (5)$$

with  $\mathbf{P} \equiv (P_1, P_2, P_3)$  and the Fermi wavelength  $\mathbf{k}_F$ . The denominator characterizes the Zeeman orbital field, whereas the numerator is related to the spin-orbit interaction. In the dual space, the spin-orbit interaction term  $h_{so}(\mathbf{k})$  is regarded as the inter-orbital in-plane anisotropic spin-orbit interaction term ( $h_{so}^{\text{dual}} = \sum_{i=1}^3 P_i(\mathbf{k}) \tilde{\sigma}^i \otimes \tilde{s}^1$ ). With increasing  $\beta$ , the in-plane spin-orbital interaction  $h_{so}^{\text{dual}}$  prevents the spin-polarization along  $z$  axis associated with the dual-space Zeeman magnetic field  $h_z^{\text{dual}}(\mathbf{k})$ . It should be noted that  $\beta$  is regarded as the indicator of the relativistic effects[28]. In the non-relativistic region ( $\beta \rightarrow 0$ ), the effective gap of the nodal topological superconductor is the spin-triplet  $p$ -wave gap with the  $\mathbf{d}$  vector  $\mathbf{d} = (v_z, 0, -v_x)$ [30]. Thus, the nodal superconductor is fragile against non-magnetic impurity in the small  $\beta$ .

Now, let us confirm the robustness numerically with the use of the self-consistent  $T$ -matrix approximation for impurities[36–39]. By considering the randomly distributed non-magnetic impurity potentials [e.g.,  $V(\mathbf{r}) = \sum_i \delta(\mathbf{r} - \mathbf{r}_i) V$ ], the  $T$ -matrix is given as  $T(\Omega) = [\mathbb{1}_8 - \frac{V}{N} \sum_{\mathbf{k}} G_{\mathbf{k}}(\Omega)]^{-1} V$  with  $V = V_0 \text{diag}(1, 1, 1, 1, -1, -1, -1, -1)$ , where  $N$  is the number of meshes in momentum space. The Green's function is

$$G_{\mathbf{k}}(\Omega) = (\Omega - \mathcal{H}(\mathbf{k}) - \Sigma(\Omega))^{-1} \equiv \begin{pmatrix} g_{\mathbf{k}}(\Omega) & f_{\mathbf{k}}(\Omega) \\ \bar{f}_{\mathbf{k}}(\Omega) & \bar{g}_{\mathbf{k}}(\Omega) \end{pmatrix}, \quad (6)$$

with the self-energy  $\Sigma(\Omega) = n_{\text{imp}} T(\Omega) - n_{\text{imp}} V$ . Here,  $n_{\text{imp}}$  denotes the impurity concentration. We study the impurity effects, checking in-gap states at the low-energy (less than gap amplitude) region in the DOS. By solving Eq.(6) self-consistently, we obtain the DOS as  $N(E) = -\frac{1}{2\pi N} \sum_{\mathbf{k}} \text{tr} [\text{Im} \lim_{\eta \rightarrow 0+} g_{\mathbf{k}}(E + i\eta)]$ . Similarly, we obtain the DOS in the normal states  $N_{\text{normal}}(E)$ , setting  $\Delta = 0$ .

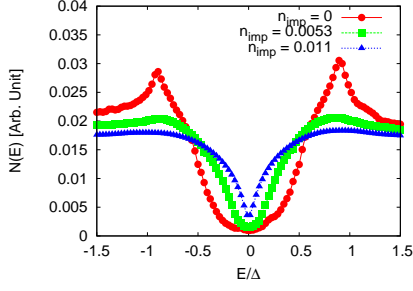


FIG. 1. (Color online) Energy dependence of the density of states  $N(E)$  in the topological gap function with point-nodes, with different impurity concentrations, in strong Zeeman orbital fields ( $\beta \sim 0.88$ ).

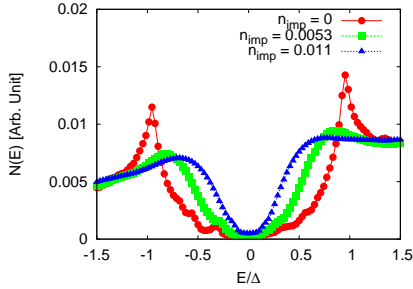


FIG. 2. (Color online) Energy dependence of the density of states  $N(E)$  in the topological gap function with point-nodes, with different impurity concentrations, in weak Zeeman orbital fields ( $\beta \sim 2.83$ ).

Let us show the setup for our numerical calculations. We adopt the large  $\mathbf{k}$ -mesh size  $N = 512^3$  in order to accurately describe point-nodes in momentum space. We focus on a unitary-like scattering model with  $V_0 = 10\text{eV}$ , to study a case that the superconducting pair is broken drastically. The gap amplitude is  $\Delta = 0.1\text{eV}$  and the smearing factor is  $\eta = 0.0025\text{eV}$ . The unit of energy is eV throughout this paper, unless otherwise noted. We set several material variables in the normal-state Hamiltonian  $h_0$ , using the data from the first-principle calculations of  $\text{Bi}_2\text{Se}_3$ . Typically, the momentum dependence of the coefficients in  $h_0$  is described by  $\epsilon(\mathbf{k}) = -\mu + \bar{D}_1\epsilon_c(\mathbf{k}) + (4/3)\bar{D}_2\epsilon_\perp(\mathbf{k})$  and  $M(\mathbf{k}) = M_0 - \bar{B}_1\epsilon_c(\mathbf{k}) - (4/3)\bar{B}_2\epsilon_\perp(\mathbf{k})$ , with  $\epsilon_c = 2 - 2\cos(k_z)$ ,  $\epsilon_\perp = 3 - 2\cos(\sqrt{3}k_x/2)\cos(k_y/2) - \cos(k_y)$ ,  $P_1(\mathbf{k}) = (2/3)\bar{A}_2\sqrt{3}\sin(\sqrt{3}k_x/2)\cos(k_y/2)$ ,  $P_2(\mathbf{k}) = (2/3)\bar{A}_2[\cos(\sqrt{3}k_x/2)\sin(k_y/2) + \sin(k_y)]$ , and  $P_3(\mathbf{k}) = A_1\sin(k_z)$ . The material variables  $\bar{D}_1$ ,  $\bar{D}_2$ ,  $\bar{B}_1$ ,  $\bar{B}_2$ ,  $\bar{A}_2$ ,

$\bar{A}_1$  are determined by the data from the first-principle calculations in Ref. 40. The remaining two quantities  $M_0$  and  $\mu$  are variable parameters in this paper, and they are closely related to the (dimensionless) strength of the Zeeman orbital field,  $\beta^{-1}$ . For simplicity, we linearize the parameter  $\beta$  as  $\beta \equiv A_2k_F/M_0 = \sqrt{(\mu/M_0)^2 - 1}$ . It should be noted that  $\beta$  is equivalent to the indicator of “relativistic” effects as shown in our previous paper[28]. The Dirac Hamiltonian has two distinct behaviors, depending on  $\beta$ : a nonrelativistic limit ( $\beta \rightarrow 0$ ) and an ultrarelativistic limit ( $\beta \rightarrow \infty$ ). We remark that the fully-gapped topological superconductivity (so-called  $\Delta_2$ [12]) has two aspects,  $p$ -wave character in a nonrelativistic limit and  $s$ -wave one in an ultrarelativistic limit, in terms of the robustness against non-magnetic impurities.

First, we show the DOS  $N(E)$  with different impurity concentrations. We use the mass and chemical potential as  $(M_0, \mu) = (0.6, 0.8)$  (*i.e.*,  $\beta \sim 0.88$ ), which is in strong Zeeman orbital field (or a nonrelativistic region). The energy dependence of the DOS without impurities has the power-law like behavior around the zero energy as shown in Fig. 1. On the other hand, 1% non-magnetic impurities induce in-gap states. This result shows that the topological superconductor with point-nodes is fragile against non-magnetic impurities in strong Zeeman orbital fields, which is similar to the topological fully-gapped superconductor[28, 41]. In weak Zeeman orbital fields (a relativistic region) as shown in Fig. 2, this superconductivity does not have the zero-energy states even with 1% impurities with the unitary-like scatters whose intensity is one-hundred times larger than the gap amplitude. Second, we calculate the impurity-concentration dependence of the ratio of the DOS in superconducting states to that in normal states. The finite DOS in the low energy indicates the Cooper pairs are broken. With increasing the indicator  $\beta$  (decreasing the Zeeman orbital field), the blue-colored region becomes large; The topological superconductors become more robust, as shown in Fig. 3. We should note that the robustness in the fully-gapped topological superconductor and the nodal topological superconductor is similar to each other. Third, we discuss the multidirectional analysis in order to confirm our claim. It should be noted that the model Hamiltonian for  $\text{CuBi}_2\text{Se}_3$  is not exactly the linearized Dirac Hamiltonian because of the existence of the higher orders of the momentum. Our claim is valid when the material can be described by the linearized massive Dirac Hamiltonian. The higher orders such as the square of the momentum might cause the different impurity effect we do not consider. In addition, it is known that the Fermi-surface evolution from the spheroidal to cylindrical shape appear with increasing the chemical potential  $\mu$ [33], which can not appear in the linearized Dirac Hamiltonian. Thus, with the use of the linearized Dirac BdG Hamiltonian around  $\Gamma$  point, we discuss the mass dependence and the chemical-potential dependence to confirm our claim. The zero-energy density of states (ZEDOS) with the fixed mass monotonically decreases with increasing the chemical po-

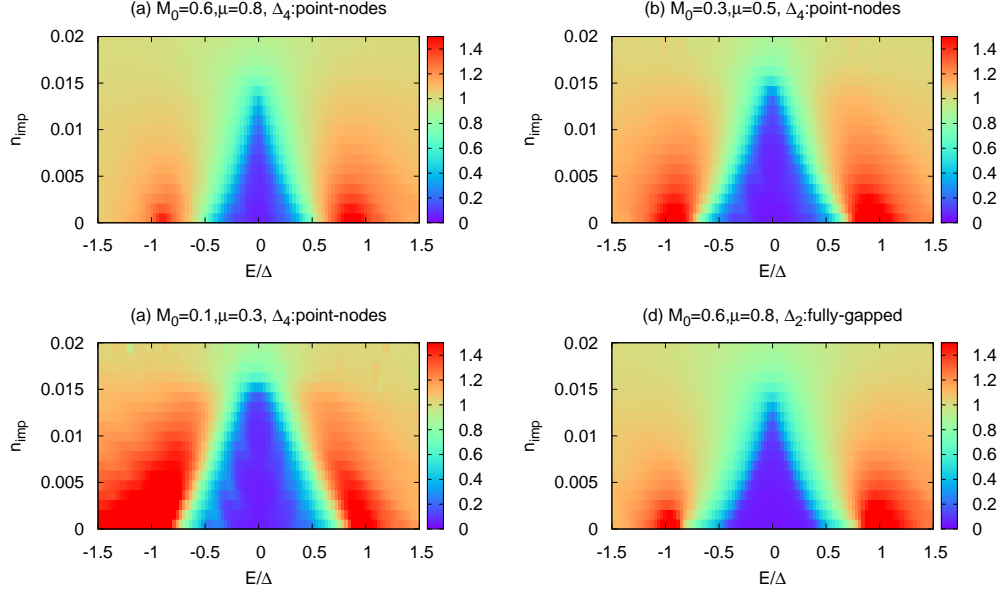


FIG. 3. (Color online) Non-magnetic impurity-concentration dependence of the ratio of the density of the states (DOS) in superconducting states to that in normal states. (a)-(c): The topological superconductors with point-nodes (so-called  $\Delta_4$ ) are considered with the different “indicator”  $\beta = \sqrt{(\mu/M_0)^2 - 1}$ . (d): The fully-gapped topological superconductivity (so-called  $\Delta_2$ ) is considered. The horizontal axis is energy  $E/\Delta$  and the vertical axis is the impurity concentration  $n_{\text{imp}}$ . The unitary-like scatterer  $V_0 = 10\text{eV}$  is adopted.

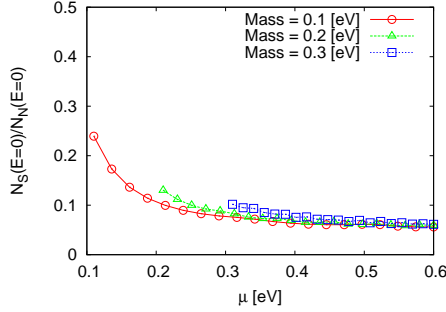


FIG. 4. (Color online) The chemical-potential dependence of the ratio of the zero-energy density of the states (DOS) in superconducting states to that in normal states, with the use of the linearized Dirac BdG Hamiltonian. The number of the meshes is  $384^3$ . The impurity concentration is  $n_{\text{imp}} = 0.02$ .

tential as shown in Fig. 4. One can also find that the ZEDOS with the fixed chemical potential monotonically decreases with decreasing the mass. These two behaviors consistent with that the indicator  $\beta = \sqrt{(\mu/M_0)^2 - 1}$  characterizes the impurity effects. We should note that the values of the ZEDOS with the fixed  $\beta$  depend on the

mass when the  $\beta$  is small. This dependence originates from the robustness in the  $\mathbf{p}$ -wave superconductors with the different mass. The kinetic term in the nonrelativistic limit depends on the mass and  $\Delta^2/M_0$  can not be neglected, which will be discussed in the future. These results show that the indicator  $\beta$ , of the relativistic effects or the Zeeman orbital fields, can well characterize the non-magnetic impurity effects.

Let us discuss the importance of the Zeeman orbital field in terms of the violation of Anderson’s theorem. Anderson’s theorem breaks down when the  $\mathbf{k}$ -averaged anomalous self-energy vanishes[23] (e.g., in  $d$ -wave and chiral  $p$ -wave superconductors). The anomalous self-energy with the non-self-consistent Born approximation is  $\Sigma_{\text{Born}}^A(\Omega) = -n_{\text{imp}}V_0^2/N \sum_{\mathbf{k}} f_{\mathbf{k}}(\Omega)$ . In our model, we obtain

$$\Sigma_{\text{Born}}^A(\Omega) = \frac{n_{\text{imp}}\Delta_4V_0^2}{N} \sum_{\mathbf{k}} \frac{C(\mathbf{k}) - (M(\mathbf{k}) + \Omega)^2}{D(\mathbf{k})}, \quad (7)$$

where  $C(\mathbf{k}) = \Delta^2 + \epsilon(\mathbf{k})^2 + P_1(\mathbf{k})^2 - P_2(\mathbf{k})^2 + P_3(\mathbf{k})^2$  and  $D(\mathbf{k}) = \det(\Omega - \mathcal{H}(\mathbf{k}))$ . We note that  $C(\mathbf{k})$  is positive and  $D(\mathbf{k})$  is strictly negative when  $\Omega$  is the Matsubara frequency ( $\Omega = i\omega_n$ ), since the  $\mathbf{k}$ -sums of  $P_1^2$  and  $P_2^2$  are same in the normal states and the spectrum of the BdG Hamiltonian is constructed by pairs of positive and negative eigenvalues, owing to its particle-hole symmetry. In zero Zeeman orbital fields (i.e.  $|M(\mathbf{k})| = 0$ ), the

anomalous self-energy never vanishes. This anomalous self-energy is very similar to that in the two-dimensional  $s$ -wave superconductor with the Zeeman magnetic fields, by replacing the Zeeman orbital field with the Zeeman magnetic field shown in Eq. (9) in Ref. 29. In strong Zeeman orbital fields ( $\beta$  in Eq. (5) is small),  $\Sigma_{\text{Born}}^A$  can be so small that the robustness dies out. Hence, the Anderson's theorem is violated, when the Zeeman orbital field is large.

In conclusion, we studied the robustness against non-magnetic impurities in the topological superconductor with point-nodes, focusing on an effective model of  $\text{Cu}_x\text{Bi}_2\text{Se}_3$ . We found that the strength of the Zeeman “orbital” field (i.e. the indicator  $\beta$ ) characterizes

the robustness, since the topological superconductor with point-nodes can be regarded as the intra-orbital spin-singlet  $s$ -wave pairing in the dual space. This strength corresponds to the weight of the relativistic effects. We showed that the topological superconductivity is not fragile in dirty materials, even with nodes. The topological superconductors can not be simply regarded as one of the *conventional* unconventional superconductors.

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